

Local vs. collective interplay of (thermal) fluctuations in polaritonic chemistry Submitting author

Monday 2 October 2023 11:05 (40 minutes)

We present recent ab-initio simulation results for matter strongly dressed by optical cavities. Our focus will be on the relevance of classical and quantum features emergent from the vibrational strong coupling to the vacuum field fluctuations at finite temperature. The role and description of cavity induced non-canonical equilibrium condition for chemical systems, as well as the relevance of thermal baths for local and collective features will be explored and consequences for the future development of ab-initio methods will be derived.

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Session Classification: Morning session